



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 03:11 PM EDT

PDB ID : 9MLC / pdb_00009mlc
EMDB ID : EMD-48353
Title : Pol II-DSIF-SPT6-PAF1c-TFIIS-IWS1-ELOF1-LEDGF-nucleosome activated elongation complex Composite map T
Authors : Syau, D.; Farnung, L.
Deposited on : 2024-12-19
Resolution : 2.40 Å (reported)
Based on initial models : 9EGZ, 6S01, 6TED

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

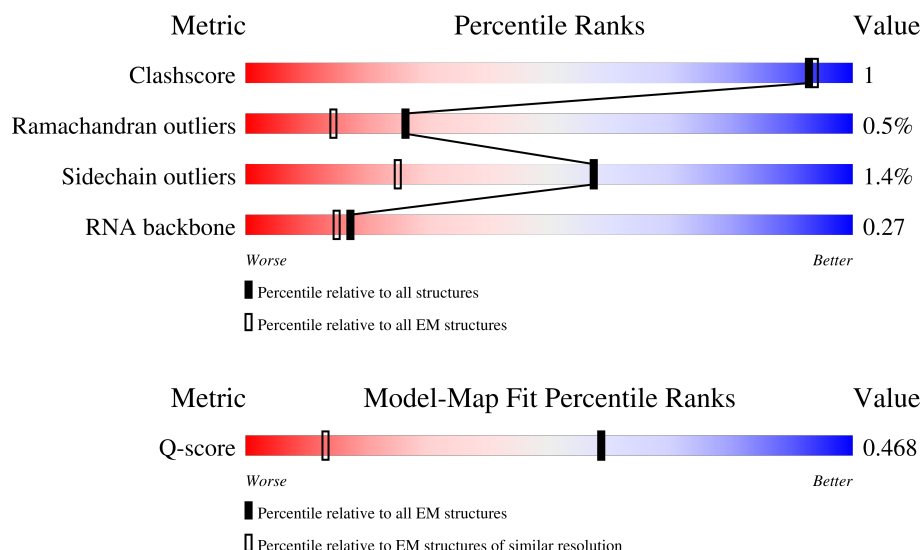
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



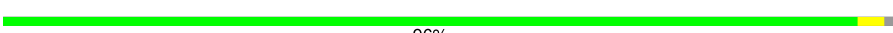
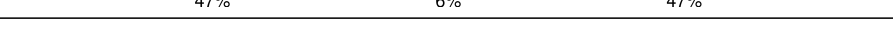
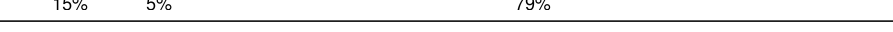
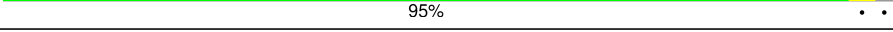
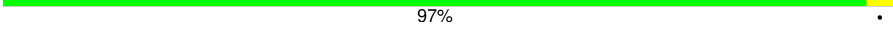
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1300	
3	C	275	

Continued on next page...

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1726	
14	N	206	
15	O	83	
16	P	39	
17	Q	1173	
18	R	710	
19	S	301	
20	T	215	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	117	
26	Z	1087	
27	i	819	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 60473 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1415	Total	C	N	O	S	0	0
			11214	7059	2006	2078	71		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9210	5817	1623	1706	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1011	637	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1341	872	216	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1198	759	195	239	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			943	582	168	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1148	Total	C	N	O	S	0	0
			7410	4465	1424	1494	27		

- Molecule 14 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	44	Total	C	N	O	P	0	0
			800	382	111	263	44		

- Molecule 15 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	67	Total	C	N	O	S	0	0
			523	322	84	110	7		

- Molecule 16 is a RNA chain called RNA (5'-R(P*UP*UP*UP*GP*GP*UP*GP*UP*GP*UP*CP*UP*GP*GP*GP*UP*GP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	20	Total	C	N	O	P	0	0
			430	190	71	149	20		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			5133	2998	1056	1068	11		

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	268	Total	C	N	O	S	0	0
			1477	832	319	323	3		

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	161	Total	C	N	O	S	0	0
			1113	657	219	230	7		

- Molecule 20 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	45	Total	C	N	O	P	0	0
			913	435	177	256	45		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	158	Total	C	N	O	S	0	0
			704	376	166	161	1		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	310	Total	C	N	O	S	0	0
			1500	826	336	335	3		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	210	Total	C	N	O	S	0	0
			1060	593	236	231			

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	117	Total	C	N	O	S	0	0
			920	575	160	175	10		

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	544	Total	C	N	O	S	0	0
			3271	1937	640	683	11		

- Molecule 27 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	229	Total	C	N	O	S	0	0
			1696	1051	313	322	10		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total 2	Zn 2	0
28	B	1	Total 1	Zn 1	0
28	C	1	Total 1	Zn 1	0
28	I	2	Total 2	Zn 2	0
28	J	1	Total 1	Zn 1	0
28	L	1	Total 1	Zn 1	0
28	S	1	Total 1	Zn 1	0
28	Y	1	Total 1	Zn 1	0

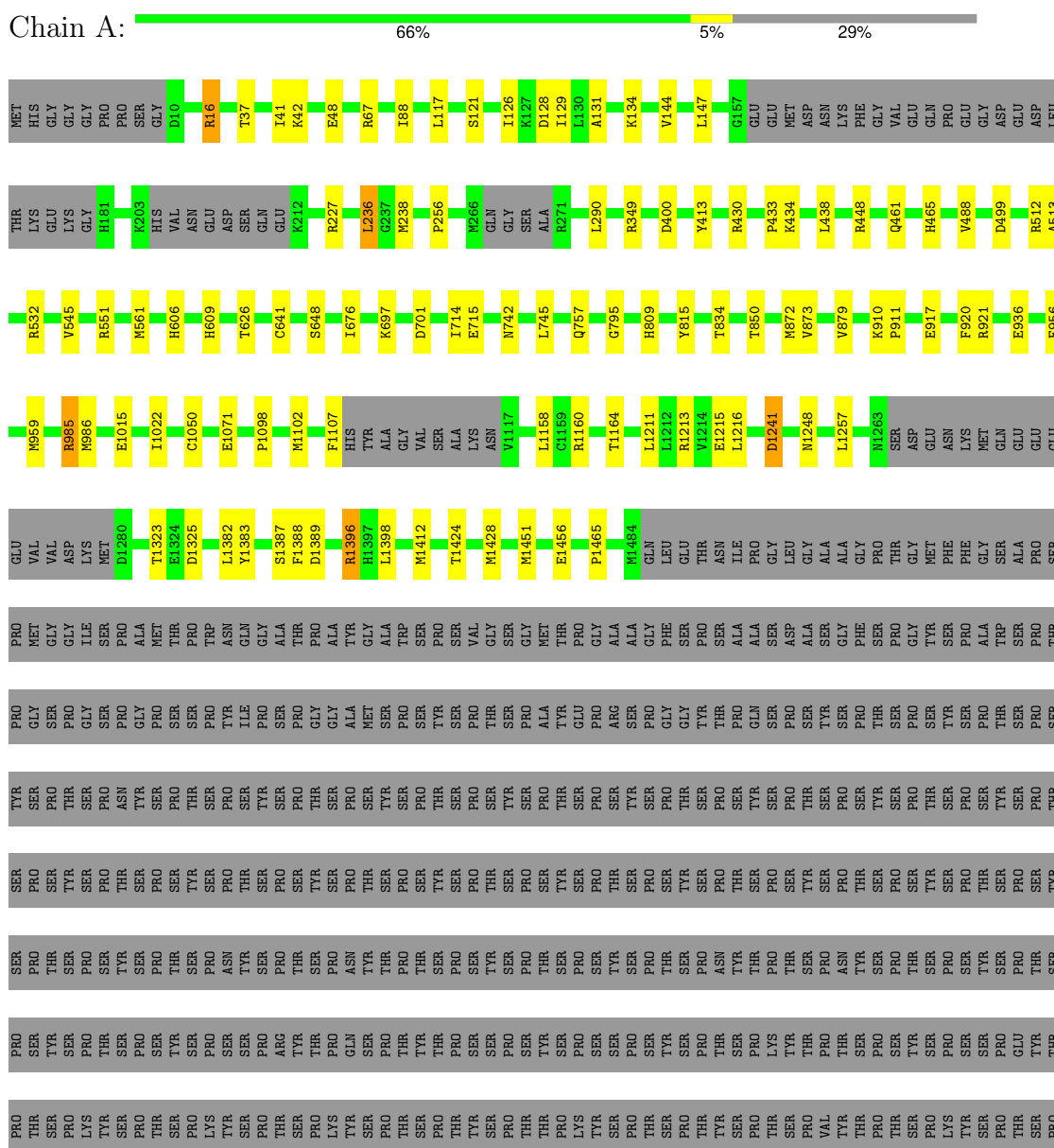
- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total 1	Mg 1	0

3 Residue-property plots

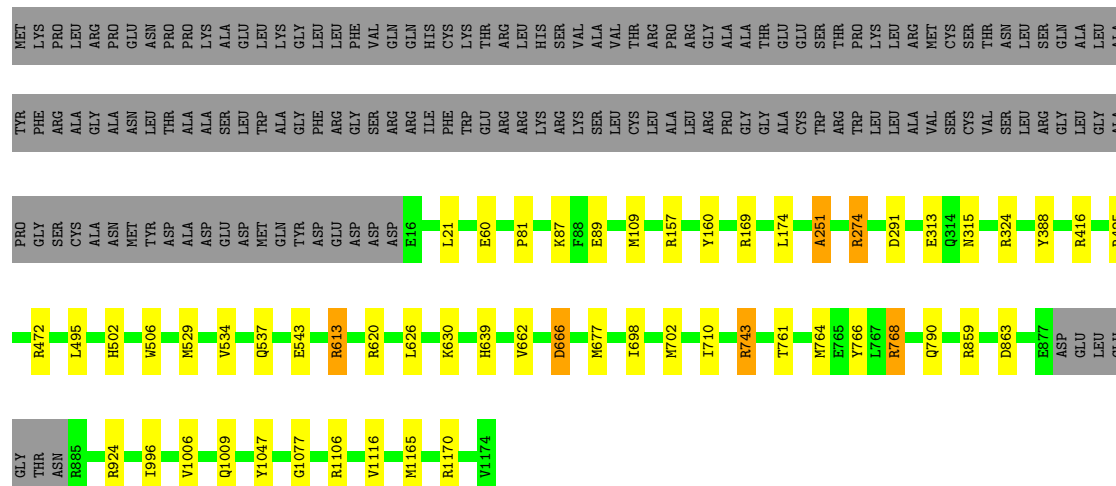
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



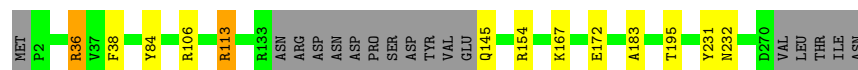
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 84% • 11%



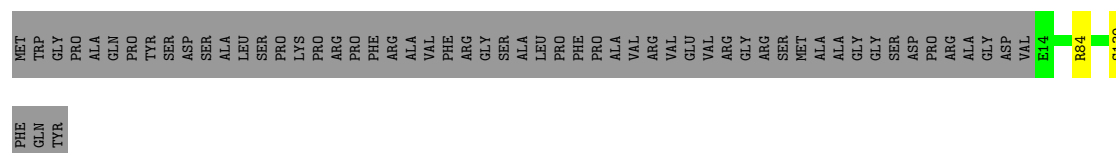
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:  89% . . 6%



- Molecule 4: RPOL4c domain-containing protein

Chain D: 67% 32%



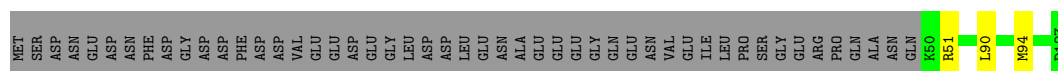
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 97%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 59% 39%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 93% 6%



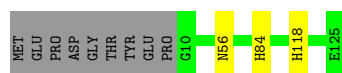
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 96%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 90% 7%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 94%



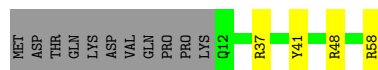
- Molecule 11: RNA polymerase II subunit J

Chain K: 95%



- Molecule 12: RNA polymerase II subunit K

Chain L: 74% 7% 19%

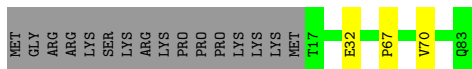
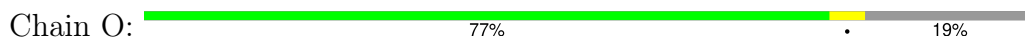


- Molecule 13: Transcription elongation factor SPT6

Chain M: 6% 64% 33%



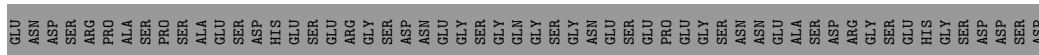
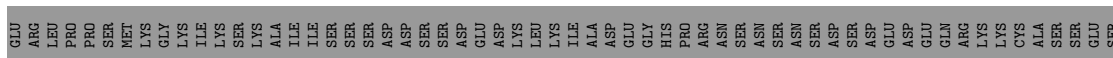
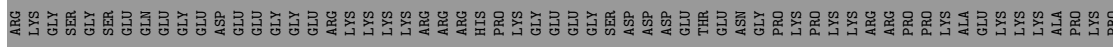
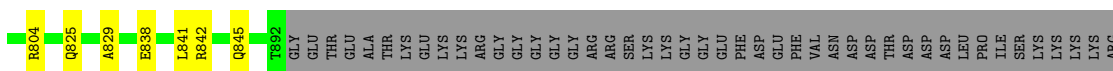
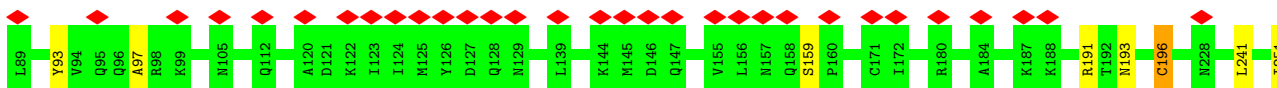
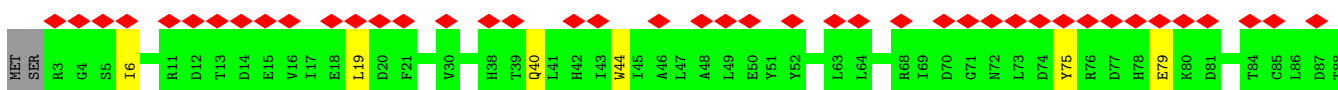
- Molecule 15: Transcription elongation factor 1 homolog



- Molecule 16: RNA (5'-R(P*UP*UP*UP*GP*GP*UP*GP*UP*GP*UP*CP*UP*GP*GP*GP*UP*GP*GP*UP*G)-3')



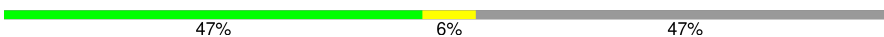
- Molecule 17: RNA polymerase-associated protein CTR9 homolog



Chain R:

[illegible]

Chain S:



ASN	ARG	ASP	THR	TYR	VAL	VAL	ARG	PHE	ALA	LYS	LYS	ASP	PRO	R132	R140	R141	R145	R148	Q171	T183	R192	R207	I215	P216	P217	D218	L219	F220	T272	T273	T274	Q275	V276	GLN	THR	ARG	SER	ALA	ASP	GLU	PRO	MET	T286	T287	V288	V289	V290	C301		
GLN	THR	SER	LEU	ALA	LYS	ARG	PHE	ILE	LEU	SER	TRP	LYS	LEU	ASP	GLY	PRO	SER	THR	GLU	LYS	ASP	GLU	LYS	LYS	GLU	PRO	ASN	ILE	THR	SER	ASN	GLN	PRO	GLU	ALA	ARG	GLU	GLY	THR	SER	VAL	ASN	ALA	ILE	ARG	LYS	GLN	THR	ASP	GLU

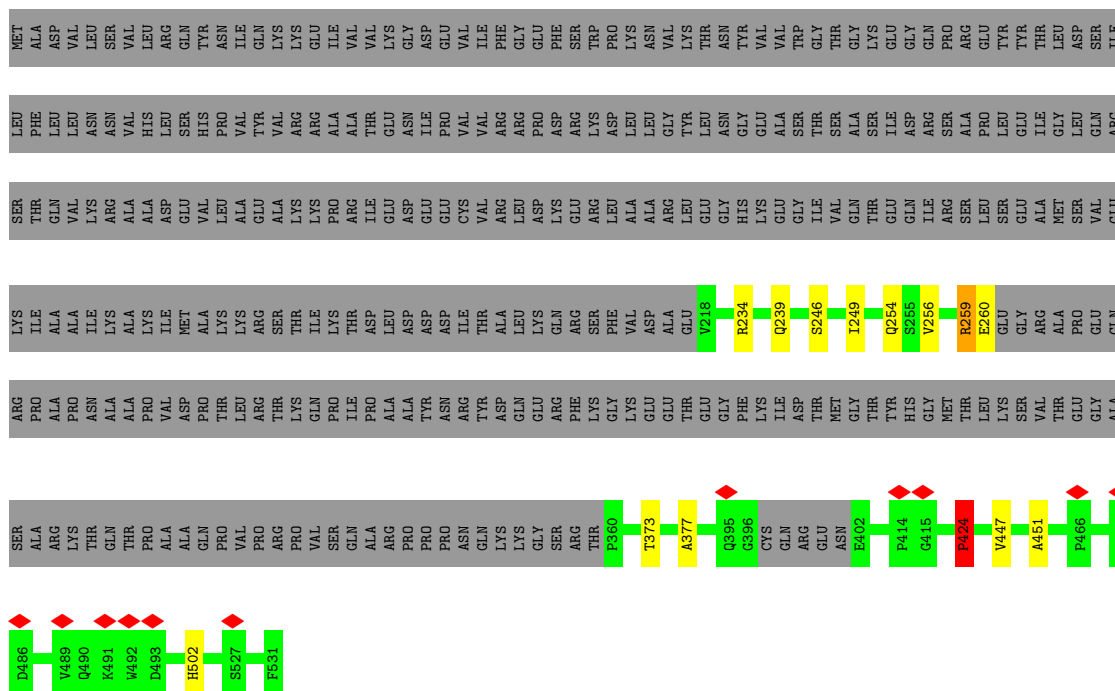
Chain T:

[illegible]



• Molecule 24: Parafibromin

Chain X: 37% 60%



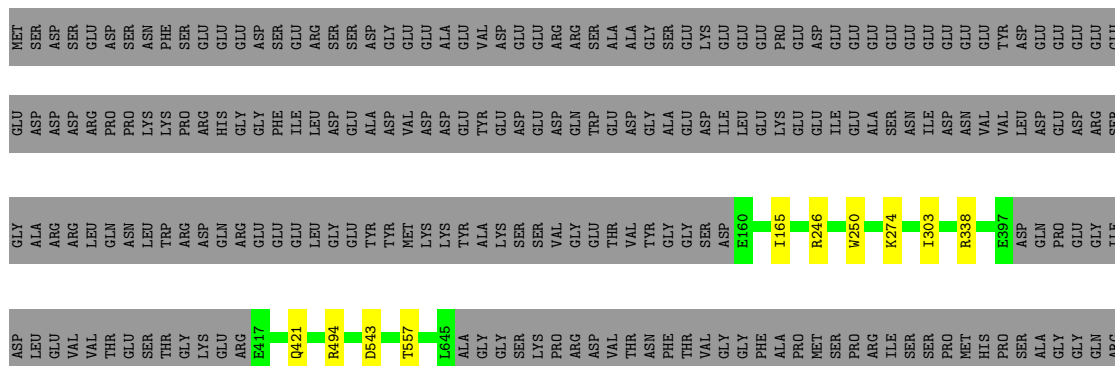
• Molecule 25: Transcription elongation factor SPT4

Chain Y: 97%



• Molecule 26: Transcription elongation factor SPT5

Chain Z: 49% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	762523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.411	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	547.4, 547.4, 547.4	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	3/11419 (0.0%)	1.16	17/15414 (0.1%)
2	B	0.79	6/9394 (0.1%)	1.32	23/12679 (0.2%)
3	C	0.76	1/2115 (0.0%)	1.31	6/2873 (0.2%)
4	D	0.81	1/1024 (0.1%)	1.28	1/1375 (0.1%)
5	E	0.73	0/1752	1.26	6/2366 (0.3%)
6	F	0.76	0/637	1.20	1/859 (0.1%)
7	G	0.69	0/1372	1.28	5/1861 (0.3%)
8	H	0.70	0/1220	1.17	2/1644 (0.1%)
9	I	0.77	0/965	1.26	1/1305 (0.1%)
10	J	0.72	0/533	1.25	0/719
11	K	0.69	1/939 (0.1%)	1.18	1/1271 (0.1%)
12	L	0.86	0/404	1.38	2/536 (0.4%)
13	M	0.75	0/7537	1.37	26/9997 (0.3%)
14	N	0.45	0/890	1.08	0/1368
15	O	0.67	0/533	1.22	1/725 (0.1%)
16	P	0.89	0/479	1.31	4/746 (0.5%)
17	Q	0.50	0/5208	0.96	11/6841 (0.2%)
18	R	0.55	0/1490	1.06	1/1941 (0.1%)
19	S	0.66	0/1120	1.15	3/1481 (0.2%)
20	T	0.52	0/1026	1.06	2/1576 (0.1%)
21	U	0.47	0/708	1.02	1/900 (0.1%)
22	V	0.51	0/1522	0.94	2/1969 (0.1%)
23	W	0.71	0/2392	1.30	4/3257 (0.1%)
24	X	0.57	1/1074 (0.1%)	1.16	5/1397 (0.4%)
25	Y	0.74	0/936	1.34	0/1260
26	Z	0.69	1/3314 (0.0%)	1.31	2/4377 (0.0%)
27	i	0.67	0/1720	1.19	6/2295 (0.3%)
All	All	0.69	14/61723 (0.0%)	1.22	133/83032 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	11
3	C	0	2
10	J	0	3
12	L	0	1
13	M	0	1
14	N	0	2
16	P	0	5
19	S	0	1
20	T	0	3
23	W	0	1
All	All	0	36

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	139	SER	C-O	-11.52	1.00	1.23
2	B	416	ARG	CZ-NH2	-9.50	1.21	1.33
1	A	512	ARG	CZ-NH2	-9.09	1.21	1.33
3	C	106	ARG	CZ-NH2	-7.13	1.24	1.33
2	B	425	ARG	CZ-NH2	-6.90	1.24	1.33
24	X	424	PRO	CG-CD	-6.85	1.27	1.50
2	B	1009	GLN	CD-NE2	-6.37	1.19	1.33
2	B	630	LYS	CE-NZ	-6.04	1.31	1.49
11	K	106	ARG	CZ-NH2	-5.64	1.26	1.33
26	Z	494	ARG	CZ-NH2	-5.33	1.26	1.33
2	B	416	ARG	CZ-NH1	-5.24	1.25	1.32
1	A	67	ARG	CZ-NH2	-5.23	1.26	1.33
2	B	1009	GLN	CD-OE1	-5.21	1.13	1.23
1	A	1215	GLU	CG-CD	-5.18	1.39	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	ALA	O-C-N	-22.69	95.42	122.19
24	X	424	PRO	N-CD-CG	-14.74	81.09	103.20
24	X	424	PRO	CA-CB-CG	-10.78	84.03	104.50
24	X	424	PRO	N-CA-CB	-8.23	93.93	103.23
1	A	1215	GLU	CB-CG-CD	7.80	125.86	112.60
2	B	1009	GLN	OE1-CD-NE2	-7.72	114.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	i	569	GLU	CB-CG-CD	7.61	125.54	112.60
13	M	995	ARG	NE-CZ-NH2	7.60	126.04	119.20
13	M	1403	GLU	N-CA-C	7.41	118.33	107.88
2	B	251	ALA	CA-C-N	7.31	130.47	120.46
2	B	251	ALA	C-N-CA	7.31	130.47	120.46
13	M	1390	ASN	N-CA-C	7.31	118.19	107.88
24	X	259	ARG	CA-C-N	-7.30	108.57	121.70
24	X	259	ARG	C-N-CA	-7.30	108.57	121.70
3	C	145	GLN	OE1-CD-NE2	-7.14	115.46	122.60
2	B	60	GLU	CB-CG-CD	7.12	124.70	112.60
17	Q	253	ASN	CA-C-N	7.04	127.75	120.00
17	Q	253	ASN	C-N-CA	7.04	127.75	120.00
16	P	29	G	O4'-C1'-N9	6.94	118.91	108.50
20	T	19	DA	C4'-C3'-O3'	6.83	120.24	110.00
22	V	37	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	1213	ARG	NE-CZ-NH2	6.66	125.19	119.20
2	B	666	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	256	PRO	N-CA-CB	6.61	106.89	103.19
2	B	537	GLN	OE1-CD-NE2	-6.38	116.22	122.60
5	E	195	ARG	NE-CZ-NH2	6.23	124.81	119.20
2	B	416	ARG	CD-NE-CZ	6.16	133.03	124.40
1	A	985	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	B	743	ARG	NE-CZ-NH2	6.07	124.66	119.20
23	W	302	ASP	CA-CB-CG	6.05	118.65	112.60
17	Q	674	ARG	NE-CZ-NH2	6.05	124.64	119.20
19	S	141	ARG	NE-CZ-NH2	5.95	124.56	119.20
26	Z	303	ILE	N-CA-C	5.87	116.08	107.75
27	i	634	ARG	NE-CZ-NH2	5.84	124.46	119.20
6	F	51	ARG	NE-CZ-NH2	5.81	124.43	119.20
13	M	297	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	551	ARG	NE-CZ-NH2	5.75	124.37	119.20
13	M	1454	LYS	CA-C-N	5.74	125.45	119.82
13	M	1454	LYS	C-N-CA	5.74	125.45	119.82
8	H	84	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	349	ARG	NE-CZ-NH2	5.74	124.37	119.20
16	P	20	G	O4'-C4'-C3'	5.74	109.74	104.00
17	Q	513	PHE	CA-CB-CG	5.73	119.53	113.80
27	i	701	ARG	NE-CZ-NH2	5.68	124.31	119.20
27	i	765	ARG	NE-CZ-NH2	5.67	124.30	119.20
19	S	192	ARG	NE-CZ-NH2	5.65	124.28	119.20
16	P	21	G	C2'-C3'-O3'	5.64	117.96	109.50
1	A	512	ARG	CD-NE-CZ	5.64	132.30	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	GLN	N-CA-C	5.63	122.25	109.81
21	U	503	LYS	O-C-N	-5.59	115.77	122.15
7	G	153	ASP	CA-CB-CG	5.59	118.19	112.60
5	E	181	ARG	NE-CZ-NH2	5.56	124.20	119.20
13	M	995	ARG	CD-NE-CZ	5.56	132.19	124.40
2	B	768	ARG	CD-NE-CZ	5.55	132.18	124.40
7	G	134	ASP	CA-CB-CG	5.55	118.15	112.60
17	Q	804	ARG	N-CA-C	5.53	117.03	109.18
5	E	66	ASP	CA-CB-CG	5.50	118.10	112.60
13	M	906	TYR	CA-C-N	5.49	123.67	119.66
13	M	906	TYR	C-N-CA	5.49	123.67	119.66
1	A	512	ARG	NH1-CZ-NH2	-5.48	112.17	119.30
17	Q	342	LEU	CA-C-N	5.48	125.19	119.82
17	Q	342	LEU	C-N-CA	5.48	125.19	119.82
13	M	368	ASN	OD1-CG-ND2	-5.48	117.12	122.60
20	T	19	DA	O5'-C5'-C4'	5.46	118.99	110.80
9	I	84	HIS	CB-CG-CD2	-5.46	124.11	131.20
26	Z	739	THR	CA-CB-CG2	5.42	119.72	110.50
1	A	88	ILE	CA-CB-CG1	5.42	119.61	110.40
12	L	58	ARG	NE-CZ-NH2	5.39	124.06	119.20
17	Q	651	ASN	OD1-CG-ND2	-5.38	117.22	122.60
8	H	11	ASP	CA-CB-CG	5.37	117.97	112.60
11	K	74	ARG	NE-CZ-NH2	5.34	124.00	119.20
3	C	154	ARG	NE-CZ-NH2	5.33	123.99	119.20
13	M	367	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	1160	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	B	1077	GLY	CA-C-N	5.31	127.66	120.38
2	B	1077	GLY	C-N-CA	5.31	127.66	120.38
2	B	291	ASP	CA-CB-CG	5.31	117.91	112.60
17	Q	585	GLN	OE1-CD-NE2	-5.30	117.30	122.60
5	E	64	HIS	CB-CG-CD2	-5.30	124.31	131.20
13	M	1399	TRP	N-CA-C	5.29	116.33	108.60
3	C	113	ARG	NE-CZ-NH2	5.29	123.96	119.20
19	S	145	ARG	NE-CZ-NH2	5.29	123.96	119.20
27	i	649	GLN	OE1-CD-NE2	-5.28	117.32	122.60
23	W	272	ASP	CA-CB-CG	5.26	117.86	112.60
13	M	995	ARG	NE-CZ-NH1	-5.25	116.25	121.50
13	M	919	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	1248	ASN	CA-CB-CG	5.24	117.84	112.60
7	G	78	ARG	NE-CZ-NH2	5.23	123.90	119.20
7	G	31	PHE	CA-CB-CG	5.21	119.01	113.80
2	B	620	ARG	NE-CZ-NH2	5.21	123.89	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	47	LYS	CA-C-N	5.21	124.66	119.24
5	E	47	LYS	C-N-CA	5.21	124.66	119.24
27	i	575	ARG	NE-CZ-NH2	5.21	123.89	119.20
13	M	409	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	C	38	PHE	CA-CB-CG	5.20	119.00	113.80
2	B	81	PRO	N-CA-CB	5.20	106.10	103.19
3	C	36	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
2	B	502	HIS	CB-CG-CD2	-5.18	124.46	131.20
16	P	20	G	C5'-C4'-C3'	-5.18	108.23	116.00
1	A	499	ASP	CA-CB-CG	5.18	117.78	112.60
12	L	48	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	B	324	ARG	NE-CZ-NH2	5.13	123.82	119.20
13	M	441	ARG	NE-CZ-NH2	5.13	123.81	119.20
4	D	84	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	448	ARG	NE-CZ-NH2	5.12	123.81	119.20
13	M	372	GLU	CA-C-N	5.12	125.34	120.43
13	M	372	GLU	C-N-CA	5.12	125.34	120.43
13	M	407	ARG	NE-CZ-NH2	5.12	123.80	119.20
23	W	271	PHE	CA-C-N	5.12	131.31	121.54
23	W	271	PHE	C-N-CA	5.12	131.31	121.54
13	M	1458	ILE	N-CA-C	5.11	113.55	107.73
18	R	467	PRO	N-CD-CG	-5.10	95.55	103.20
3	C	172	GLU	N-CA-CB	5.09	117.79	110.20
22	V	124	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	B	639	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	B	924	ARG	NE-CZ-NH2	5.09	123.78	119.20
13	M	1416	VAL	N-CA-C	5.09	116.42	110.62
1	A	227	ARG	NE-CZ-NH2	5.08	123.78	119.20
17	Q	702	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	742	ASN	CA-CB-CG	5.08	117.67	112.60
15	O	32	GLU	N-CA-C	5.08	117.55	111.71
2	B	169	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	B	274	ARG	NE-CZ-NH1	-5.07	116.43	121.50
13	M	907	PRO	N-CA-CB	5.07	106.03	103.19
2	B	613	ARG	NE-CZ-NH2	5.06	123.76	119.20
13	M	1417	GLN	CA-C-N	5.06	124.85	119.28
13	M	1417	GLN	C-N-CA	5.06	124.85	119.28
13	M	1067	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	16	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	B	1170	ARG	NE-CZ-NH2	5.04	123.74	119.20
17	Q	341	VAL	N-CA-C	5.03	115.25	110.42
7	G	4	HIS	CA-CB-CG	5.00	118.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	380	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396	ARG	Sidechain
1	A	413	TYR	Sidechain
1	A	430	ARG	Sidechain
1	A	532	ARG	Sidechain
1	A	815	TYR	Sidechain
1	A	985	ARG	Sidechain
2	B	1047	TYR	Sidechain
2	B	1106	ARG	Sidechain
2	B	157	ARG	Sidechain
2	B	160	TYR	Sidechain
2	B	251	ALA	Mainchain
2	B	274	ARG	Sidechain
2	B	472	ARG	Sidechain
2	B	613	ARG	Sidechain
2	B	743	ARG	Sidechain
2	B	766	TYR	Sidechain
2	B	859	ARG	Sidechain
3	C	113	ARG	Sidechain
3	C	231	TYR	Sidechain
10	J	47	ARG	Sidechain
10	J	6	ARG	Sidechain
10	J	62	TYR	Sidechain
12	L	41	TYR	Sidechain
13	M	301	ARG	Sidechain
14	N	-7	DT	Sidechain
14	N	7	DG	Sidechain
16	P	21	G	Sidechain
16	P	25	G	Sidechain
16	P	26	U	Sidechain
16	P	34	G	Sidechain
16	P	35	U	Sidechain
19	S	207	ARG	Sidechain
20	T	-2	DG	Sidechain
20	T	19	DA	Sidechain
20	T	6	DC	Sidechain
23	W	213	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	11344	43	0
2	B	9210	0	9231	12	0
3	C	2072	0	2019	4	0
4	D	1011	0	994	0	0
5	E	1721	0	1737	0	0
6	F	627	0	657	1	0
7	G	1341	0	1343	1	0
8	H	1198	0	1156	0	0
9	I	943	0	871	0	0
10	J	524	0	540	0	0
11	K	920	0	942	5	0
12	L	398	0	401	0	0
13	M	7410	0	5973	2	0
14	N	800	0	446	14	0
15	O	523	0	484	0	0
16	P	430	0	212	0	0
17	Q	5133	0	3642	41	0
18	R	1477	0	982	0	0
19	S	1113	0	997	10	0
20	T	913	0	500	6	0
21	U	704	0	307	1	0
22	V	1500	0	767	6	0
23	W	2333	0	2246	2	0
24	X	1060	0	627	13	0
25	Y	920	0	916	0	0
26	Z	3271	0	2547	8	0
27	i	1696	0	1653	6	0
28	A	2	0	0	0	0
28	B	1	0	0	0	0
28	C	1	0	0	0	0
28	I	2	0	0	0	0
28	J	1	0	0	0	0
28	L	1	0	0	0	0
28	S	1	0	0	0	0
28	Y	1	0	0	0	0
29	A	1	0	0	0	0
All	All	60473	0	53534	157	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:259:ARG:O	24:X:259:ARG:NE	1.93	1.01
14:N:-15:DC:OP2	26:Z:250:TRP:CZ2	2.34	0.81
14:N:-8:DG:H2''	14:N:-7:DT:H5'	1.64	0.80
27:i:556:ALA:HB1	27:i:606:THR:HG21	1.70	0.73
22:V:42:ILE:HD12	22:V:42:ILE:H	1.54	0.72
2:B:506:TRP:CH2	2:B:677:MET:HE1	2.26	0.71
14:N:-15:DC:H5'	26:Z:250:TRP:CZ2	2.26	0.70
14:N:-15:DC:OP2	26:Z:250:TRP:CE2	2.46	0.69
24:X:259:ARG:O	24:X:259:ARG:CZ	2.41	0.68
14:N:-15:DC:OP2	26:Z:250:TRP:NE1	2.27	0.68
24:X:259:ARG:O	24:X:259:ARG:NH1	2.29	0.66
1:A:917:GLU:OE2	1:A:921:ARG:NH2	2.30	0.65
19:S:132:ARG:O	19:S:132:ARG:NH2	2.28	0.65
14:N:16:DT:O2	20:T:-14:DG:N2	2.30	0.65
1:A:1241:ASP:OD1	1:A:1241:ASP:N	2.31	0.63
14:N:-15:DC:OP2	26:Z:250:TRP:HZ2	1.79	0.62
14:N:-8:DG:H2''	14:N:-7:DT:C5'	2.28	0.62
17:Q:677:THR:HG22	17:Q:679:ASP:H	1.64	0.62
24:X:424:PRO:O	24:X:424:PRO:HG2	1.99	0.62
1:A:121:SER:HA	1:A:126:ILE:HG21	1.82	0.61
19:S:272:THR:O	19:S:290:VAL:N	2.29	0.61
3:C:36:ARG:NH2	11:K:41:THR:HG23	2.16	0.60
20:T:-9:DA:H2'	20:T:-8:DT:C6	2.36	0.60
24:X:259:ARG:HE	24:X:259:ARG:C	2.09	0.60
22:V:357:ASN:O	22:V:361:LEU:N	2.33	0.59
19:S:215:ILE:HD12	19:S:215:ILE:O	2.03	0.59
17:Q:40:GLN:O	17:Q:44:TRP:N	2.35	0.58
1:A:434:LYS:CD	1:A:434:LYS:H	2.15	0.58
17:Q:653:ILE:O	17:Q:657:LEU:HD13	2.04	0.58
1:A:1383:TYR:O	1:A:1387:SER:OG	2.20	0.58
17:Q:838:GLU:O	17:Q:842:ARG:N	2.34	0.58
1:A:561:MET:HE1	11:K:51:LEU:HD21	1.87	0.56
3:C:36:ARG:HH21	11:K:41:THR:HG23	1.70	0.56
17:Q:449:VAL:O	17:Q:480:ARG:NE	2.40	0.55
2:B:996:ILE:HG12	22:V:134:THR:HG22	1.89	0.55
2:B:529:MET:HE2	2:B:702:MET:HG3	1.88	0.55
17:Q:750:ASP:HB3	17:Q:753:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:643:ASP:OD2	24:X:239:GLN:NE2	2.35	0.55
23:W:110:TRP:CG	23:W:111:THR:H	2.25	0.55
24:X:373:THR:O	24:X:377:ALA:N	2.39	0.54
1:A:433:PRO:HG2	1:A:438:LEU:HD21	1.90	0.54
17:Q:841:LEU:O	17:Q:845:GLN:N	2.36	0.54
17:Q:404:VAL:O	17:Q:408:TYR:N	2.41	0.54
14:N:-15:DC:OP1	26:Z:246:ARG:NH2	2.41	0.53
1:A:834:THR:HG23	2:B:677:MET:HE3	1.90	0.53
1:A:920:PHE:HB3	1:A:959:MET:HE3	1.91	0.53
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.26	0.53
2:B:529:MET:HE1	2:B:698:ILE:HD12	1.91	0.53
17:Q:592:LEU:HD12	17:Q:603:SER:HB3	1.91	0.52
17:Q:594:GLN:NE2	17:Q:596:SER:OG	2.40	0.52
2:B:710:ILE:HA	2:B:764:MET:HE2	1.91	0.52
20:T:-15:DA:H2''	20:T:-14:DG:C8	2.45	0.52
27:i:650:GLU:HB3	27:i:654:HIS:CE1	2.45	0.52
17:Q:621:ASP:OD1	17:Q:622:ARG:NH2	2.42	0.51
14:N:-16:DT:H3'	26:Z:250:TRP:HE1	1.73	0.51
1:A:545:VAL:HG12	1:A:676:ILE:HG13	1.92	0.51
19:S:218:ASP:N	19:S:218:ASP:OD1	2.43	0.51
17:Q:592:LEU:O	17:Q:597:THR:OG1	2.29	0.51
24:X:254:GLN:HA	24:X:254:GLN:OE1	2.12	0.50
17:Q:619:THR:OG1	17:Q:622:ARG:NH2	2.44	0.50
23:W:110:TRP:CD1	23:W:111:THR:H	2.29	0.50
24:X:259:ARG:NE	24:X:259:ARG:C	2.65	0.50
22:V:42:ILE:HD12	22:V:42:ILE:N	2.25	0.50
24:X:249:ILE:HD12	24:X:249:ILE:H	1.76	0.50
17:Q:526:GLU:OE2	17:Q:527:HIS:NE2	2.45	0.50
17:Q:524:LEU:HD21	17:Q:533:CYS:HB3	1.93	0.49
1:A:48:GLU:O	1:A:48:GLU:CD	2.54	0.49
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.95	0.49
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.93	0.49
27:i:608:ILE:HD12	27:i:609:ASP:N	2.28	0.49
17:Q:825:GLN:O	17:Q:829:ALA:N	2.41	0.49
1:A:795:GLY:HA2	1:A:1107:PHE:CD2	2.48	0.48
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.48	0.48
1:A:434:LYS:H	1:A:434:LYS:HD2	1.76	0.48
24:X:239:GLN:OE1	24:X:239:GLN:HA	2.13	0.48
24:X:246:SER:O	24:X:249:ILE:HD12	2.14	0.48
1:A:131:ALA:HA	1:A:134:LYS:HE2	1.96	0.48
2:B:506:TRP:CZ2	2:B:677:MET:HE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:LYS:N	1:A:911:PRO:HD2	2.30	0.47
20:T:-8:DT:H2"	20:T:-7:DA:H8	1.79	0.47
1:A:697:LYS:NZ	1:A:701:ASP:OD1	2.48	0.47
22:V:42:ILE:H	22:V:42:ILE:CD1	2.25	0.47
19:S:140:VAL:HG11	19:S:183:THR:HG21	1.96	0.47
1:A:1424:THR:HB	1:A:1428:MET:SD	2.55	0.46
1:A:117:LEU:HD21	1:A:236:LEU:CD1	2.46	0.46
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.31	0.46
27:i:561:SER:O	27:i:564:ILE:HG22	2.15	0.46
19:S:216:PRO:O	19:S:219:LEU:CD1	2.64	0.46
17:Q:657:LEU:HA	17:Q:660:LYS:HB2	1.98	0.46
1:A:1389:ASP:N	1:A:1389:ASP:OD1	2.49	0.45
17:Q:594:GLN:O	17:Q:598:GLN:N	2.49	0.45
27:i:560:VAL:HG21	27:i:606:THR:HG23	1.97	0.45
1:A:37:THR:HG21	1:A:41:ILE:HD11	1.99	0.45
17:Q:473:TYR:O	17:Q:477:SER:N	2.36	0.45
17:Q:767:SER:O	17:Q:770:LYS:HG3	2.17	0.45
7:G:130:THR:HG22	7:G:135:ILE:H	1.82	0.45
17:Q:284:ASP:O	17:Q:288:VAL:N	2.43	0.45
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.99	0.45
17:Q:75:TYR:O	17:Q:79:GLU:N	2.43	0.44
20:T:-12:DT:H2"	20:T:-11:DA:C8	2.52	0.44
1:A:986:MET:HE2	1:A:1071:GLU:HG3	1.99	0.44
1:A:126:ILE:HD11	1:A:144:VAL:HG22	2.00	0.44
1:A:128:ASP:OD1	1:A:129:ILE:N	2.50	0.44
1:A:561:MET:HE1	11:K:51:LEU:CD2	2.47	0.44
2:B:761:THR:H	2:B:764:MET:HE3	1.83	0.44
17:Q:728:PHE:HZ	17:Q:763:ARG:HD3	1.82	0.44
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.85	0.43
19:S:219:LEU:HD12	19:S:220:PHE:N	2.33	0.43
2:B:109:MET:HE2	2:B:174:LEU:HD13	2.00	0.43
1:A:1456:GLU:OE1	1:A:1456:GLU:N	2.44	0.43
19:S:274:THR:O	19:S:288:PHE:N	2.41	0.43
14:N:-17:DG:H4'	14:N:-16:DT:OP1	2.18	0.43
2:B:1006:VAL:HG22	22:V:130:TRP:CG	2.54	0.43
1:A:513:ALA:HB2	6:F:90:LEU:HD11	2.00	0.42
1:A:1388:PHE:CD1	1:A:1388:PHE:C	2.97	0.42
1:A:1098:PRO:O	1:A:1102:MET:HG3	2.19	0.42
17:Q:492:TYR:CD1	17:Q:492:TYR:C	2.97	0.42
17:Q:592:LEU:HD12	17:Q:603:SER:CB	2.49	0.42
1:A:1216:LEU:H	1:A:1216:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:434:TYR:O	17:Q:438:THR:N	2.44	0.42
17:Q:93:TYR:O	17:Q:97:ALA:N	2.51	0.42
1:A:872:MET:HE1	1:A:1465:PRO:O	2.18	0.42
17:Q:615:LEU:C	17:Q:615:LEU:HD13	2.45	0.42
17:Q:736:CYS:O	17:Q:740:LEU:HB2	2.19	0.42
26:Z:725:LYS:HE3	26:Z:735:GLU:CD	2.45	0.42
17:Q:6:ILE:N	17:Q:19:LEU:O	2.52	0.42
1:A:1382:LEU:HB3	1:A:1398:LEU:HD21	2.01	0.42
17:Q:564:HIS:CE1	17:Q:566:ASP:HB2	2.55	0.42
20:T:2:DA:H2'	20:T:3:DT:H71	2.01	0.41
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.55	0.41
1:A:921:ARG:HD3	1:A:956:PHE:CD2	2.56	0.41
17:Q:485:ALA:HA	17:Q:492:TYR:CE2	2.54	0.41
17:Q:251:ILE:O	17:Q:255:VAL:N	2.42	0.41
27:i:710:GLU:O	27:i:713:PRO:HD3	2.20	0.41
17:Q:191:ARG:N	17:Q:196:CYS:O	2.54	0.41
21:U:521:LEU:H	21:U:521:LEU:HD22	1.85	0.41
17:Q:558:LEU:HD11	17:Q:568:TRP:CE2	2.55	0.41
1:A:42:LYS:HB2	1:A:42:LYS:HE2	1.75	0.41
13:M:756:ALA:HB3	13:M:1140:ALA:HA	2.02	0.41
14:N:-27:DT:H4'	14:N:-26:DG:OP1	2.19	0.41
19:S:171:GLN:OE1	19:S:217:PRO:HB2	2.21	0.41
1:A:434:LYS:CD	1:A:434:LYS:N	2.83	0.41
13:M:469:LEU:HD13	13:M:469:LEU:C	2.46	0.41
14:N:-22:DG:H8	14:N:-22:DG:P	2.43	0.41
14:N:-8:DG:H3'	14:N:-8:DG:OP2	2.21	0.41
17:Q:728:PHE:CZ	17:Q:763:ARG:HD3	2.56	0.41
1:A:1451:MET:HE3	1:A:1451:MET:HB3	1.84	0.41
17:Q:535:LEU:HA	17:Q:535:LEU:HD12	1.80	0.41
19:S:216:PRO:HD2	19:S:219:LEU:HD21	2.02	0.41
1:A:809:HIS:CG	2:B:677:MET:HE2	2.56	0.40
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.78	0.40
17:Q:475:LEU:HD13	17:Q:475:LEU:HA	1.87	0.40
17:Q:480:ARG:HH22	17:Q:484:GLU:CD	2.29	0.40
17:Q:522:ASN:HA	17:Q:525:ARG:HG2	2.03	0.40
24:X:256:VAL:O	24:X:260:GLU:N	2.42	0.40
1:A:238:MET:HE2	1:A:238:MET:HB3	1.85	0.40
1:A:1022:ILE:HD13	1:A:1022:ILE:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1403/1984 (71%)	1358 (97%)	45 (3%)	0	100	100
2	B	1148/1300 (88%)	1095 (95%)	52 (4%)	1 (0%)	48	64
3	C	254/275 (92%)	249 (98%)	5 (2%)	0	100	100
4	D	124/184 (67%)	120 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	32
8	H	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
9	I	114/125 (91%)	107 (94%)	6 (5%)	1 (1%)	14	22
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	45/58 (78%)	43 (96%)	2 (4%)	0	100	100
13	M	1130/1726 (66%)	1063 (94%)	51 (4%)	16 (1%)	9	13
15	O	65/83 (78%)	65 (100%)	0	0	100	100
17	Q	888/1173 (76%)	829 (93%)	50 (6%)	9 (1%)	12	20
18	R	264/710 (37%)	248 (94%)	16 (6%)	0	100	100
19	S	157/301 (52%)	147 (94%)	10 (6%)	0	100	100
21	U	148/666 (22%)	126 (85%)	20 (14%)	2 (1%)	9	13
22	V	302/531 (57%)	253 (84%)	45 (15%)	4 (1%)	9	14
23	W	298/305 (98%)	269 (90%)	26 (9%)	3 (1%)	12	20
24	X	204/531 (38%)	176 (86%)	25 (12%)	3 (2%)	8	12
25	Y	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
26	Z	536/1087 (49%)	510 (95%)	22 (4%)	4 (1%)	18	28
27	i	219/819 (27%)	211 (96%)	8 (4%)	0	100	100
All	All	8190/12818 (64%)	7735 (94%)	411 (5%)	44 (0%)	26	37

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	846	HIS
13	M	854	ASN
13	M	1330	ILE
13	M	1398	LEU
13	M	1407	ASP
17	Q	159	SER
17	Q	193	ASN
17	Q	241	LEU
17	Q	342	LEU
22	V	196	LYS
22	V	226	ASP
24	X	447	VAL
26	Z	543	ASP
17	Q	196	CYS
17	Q	412	VAL
7	G	116	GLU
13	M	221	PHE
13	M	336	CYS
13	M	844	LYS
13	M	1404	GLU
17	Q	712	TYR
23	W	272	ASP
24	X	502	HIS
2	B	790	GLN
13	M	1415	TYR
13	M	1454	LYS
13	M	1479	ARG
17	Q	546	ASN
21	U	522	PRO
23	W	221	HIS
26	Z	274	LYS
26	Z	338	ARG
26	Z	557	THR
13	M	692	PHE
13	M	696	ASP
13	M	1077	ASP
17	Q	732	LYS
21	U	450	LEU
22	V	59	VAL
23	W	149	LYS
24	X	451	ALA
9	I	118	HIS

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Mol	Chain	Res	Type
22	V	207	VAL
13	M	384	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1246/1763 (71%)	1224 (98%)	22 (2%)	51	73
2	B	1007/1127 (89%)	993 (99%)	14 (1%)	59	79
3	C	235/252 (93%)	234 (100%)	1 (0%)	84	92
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	67 (98%)	1 (2%)	57	77
7	G	148/153 (97%)	145 (98%)	3 (2%)	48	70
8	H	130/131 (99%)	127 (98%)	3 (2%)	44	66
9	I	104/112 (93%)	103 (99%)	1 (1%)	68	84
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	43 (98%)	1 (2%)	44	66
13	M	597/1522 (39%)	591 (99%)	6 (1%)	68	84
15	O	61/76 (80%)	59 (97%)	2 (3%)	33	55
17	Q	327/1005 (32%)	322 (98%)	5 (2%)	57	77
18	R	86/623 (14%)	84 (98%)	2 (2%)	44	66
19	S	102/266 (38%)	101 (99%)	1 (1%)	68	84
21	U	18/590 (3%)	16 (89%)	2 (11%)	6	9
22	V	62/462 (13%)	61 (98%)	1 (2%)	55	76
23	W	255/260 (98%)	252 (99%)	3 (1%)	63	81
24	X	53/467 (11%)	51 (96%)	2 (4%)	29	49
25	Y	103/103 (100%)	100 (97%)	3 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Z	250/940 (27%)	247 (99%)	3 (1%)	63	81
27	i	175/736 (24%)	173 (99%)	2 (1%)	65	82
All	All	5530/11268 (49%)	5452 (99%)	78 (1%)	57	79

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	236	LEU
1	A	290	LEU
1	A	400	ASP
1	A	465	HIS
1	A	488	VAL
1	A	648	SER
1	A	714	ILE
1	A	715	GLU
1	A	745	LEU
1	A	757	GLN
1	A	850	THR
1	A	936	GLU
1	A	1015	GLU
1	A	1050	CYS
1	A	1158	LEU
1	A	1164	THR
1	A	1211	LEU
1	A	1241	ASP
1	A	1257	LEU
1	A	1396	ARG
1	A	1412	MET
2	B	21	LEU
2	B	87	LYS
2	B	89	GLU
2	B	313	GLU
2	B	315	ASN
2	B	388	TYR
2	B	495	LEU
2	B	534	VAL
2	B	543	GLU
2	B	666	ASP
2	B	768	ARG
2	B	863	ASP

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Mol	Chain	Res	Type
2	B	1116	VAL
2	B	1165	MET
3	C	195	THR
6	F	94	MET
7	G	92	VAL
7	G	160	ILE
7	G	167	TYR
8	H	7	GLU
8	H	32	SER
8	H	74	GLU
9	I	56	ASN
12	L	37	ARG
13	M	331	SER
13	M	366	MET
13	M	550	LEU
13	M	571	LYS
13	M	900	GLU
13	M	1154	THR
15	O	67	PRO
15	O	70	VAL
17	Q	597	THR
17	Q	687	LEU
17	Q	702	GLN
17	Q	733	LEU
17	Q	741	LEU
18	R	520	LYS
18	R	557	ILE
19	S	148	LEU
21	U	519	ARG
21	U	521	LEU
22	V	139	THR
23	W	73	SER
23	W	238	VAL
23	W	240	PHE
24	X	234	ARG
24	X	424	PRO
25	Y	17	LEU
25	Y	22	VAL
25	Y	53	THR
26	Z	165	ILE
26	Z	421	GLN
26	Z	740	CYS

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Mol	Chain	Res	Type
27	i	585	LEU
27	i	647	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	72	GLN
1	A	504	HIS
1	A	673	GLN
1	A	678	ASN
1	A	723	ASN
1	A	765	ASN
1	A	783	GLN
1	A	825	ASN
1	A	1172	ASN
1	A	1236	ASN
2	B	188	ASN
2	B	420	GLN
2	B	642	GLN
2	B	717	ASN
2	B	722	ASN
2	B	725	GLN
2	B	1025	ASN
2	B	1049	GLN
2	B	1068	GLN
2	B	1071	ASN
3	C	18	ASN
3	C	55	ASN
3	C	190	ASN
3	C	217	GLN
3	C	232	ASN
4	D	19	GLN
4	D	47	GLN
5	E	168	ASN
7	G	53	ASN
7	G	139	GLN
8	H	87	GLN
9	I	45	GLN
9	I	84	HIS
9	I	91	HIS
9	I	118	HIS

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Mol	Chain	Res	Type
11	K	29	ASN
11	K	36	ASN
12	L	13	GLN
13	M	466	HIS
13	M	480	ASN
13	M	528	GLN
13	M	595	GLN
13	M	731	ASN
13	M	999	HIS
13	M	1008	ASN
13	M	1016	GLN
17	Q	594	GLN
17	Q	762	GLN
18	R	584	HIS
22	V	148	ASN
23	W	57	GLN
23	W	95	ASN
23	W	119	GLN
23	W	173	ASN
23	W	184	HIS
23	W	276	GLN
23	W	285	ASN
25	Y	75	GLN
26	Z	211	GLN
26	Z	232	GLN
26	Z	237	GLN
26	Z	244	ASN
26	Z	251	ASN
26	Z	446	ASN
27	i	578	ASN
27	i	654	HIS
27	i	711	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	19/39 (48%)	8 (42%)	2 (10%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	19	U
16	P	21	G
16	P	22	U
16	P	23	G
16	P	24	U
16	P	27	C
16	P	34	G
16	P	35	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	22	U
16	P	34	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

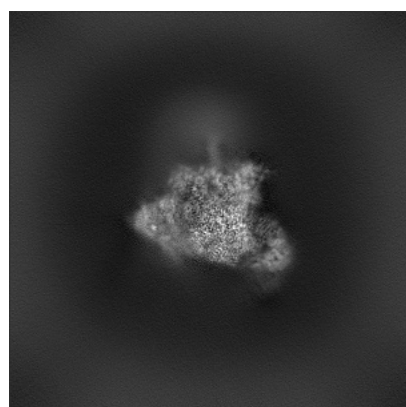
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48353. These allow visual inspection of the internal detail of the map and identification of artifacts.

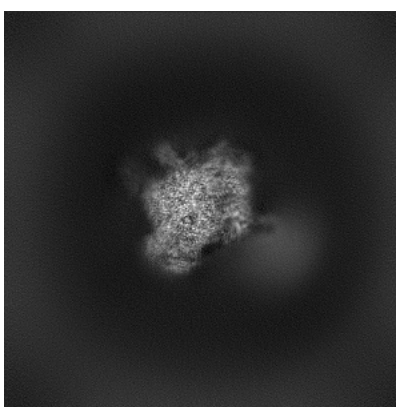
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

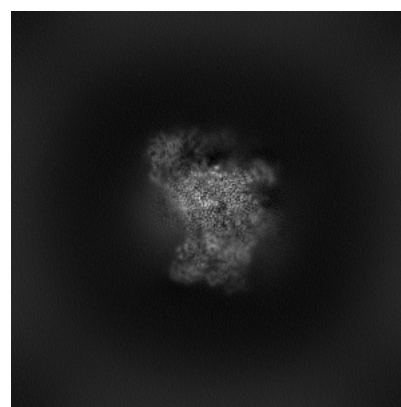
6.1.1 Primary map



X



Y

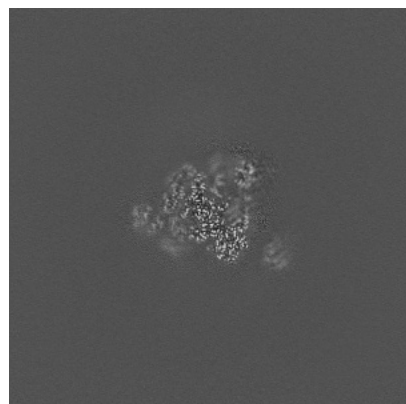


Z

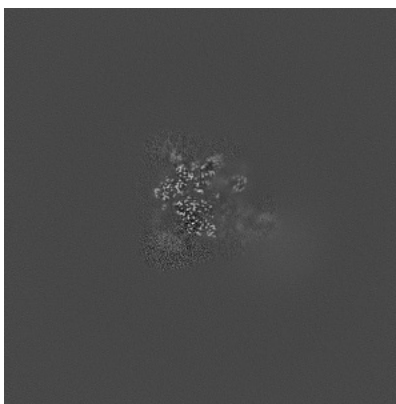
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

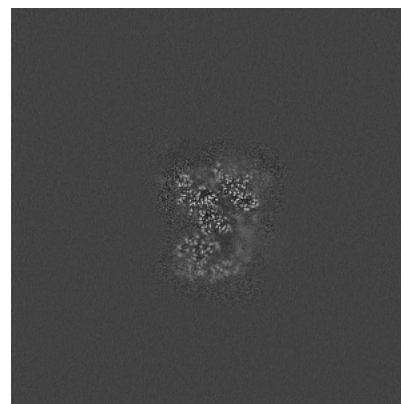
6.2.1 Primary map



X Index: 230



Y Index: 230

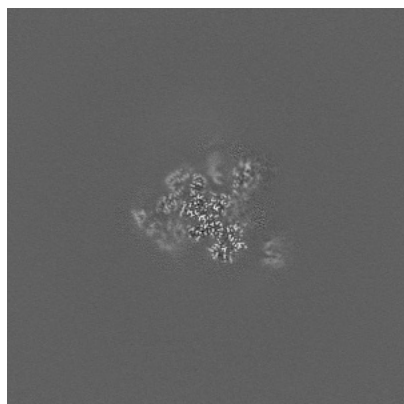


Z Index: 230

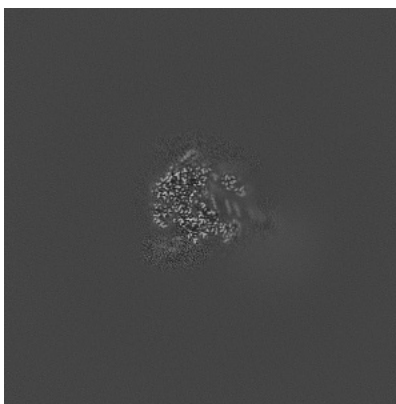
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

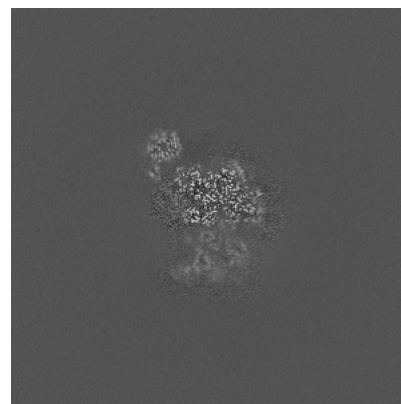
6.3.1 Primary map



X Index: 227



Y Index: 244

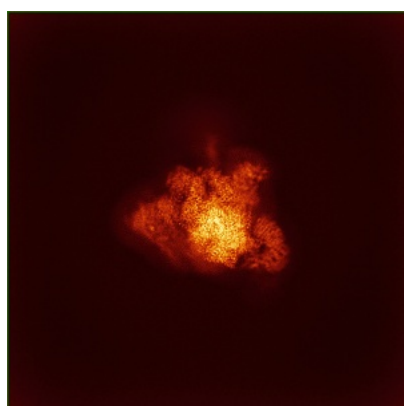


Z Index: 204

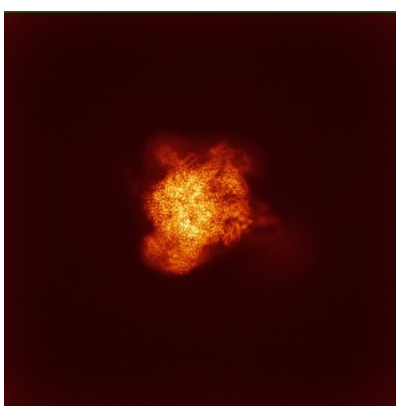
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

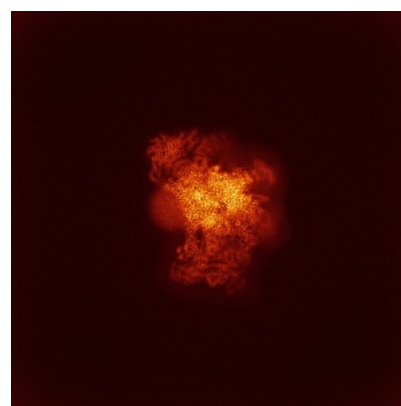
6.4.1 Primary map



X



Y

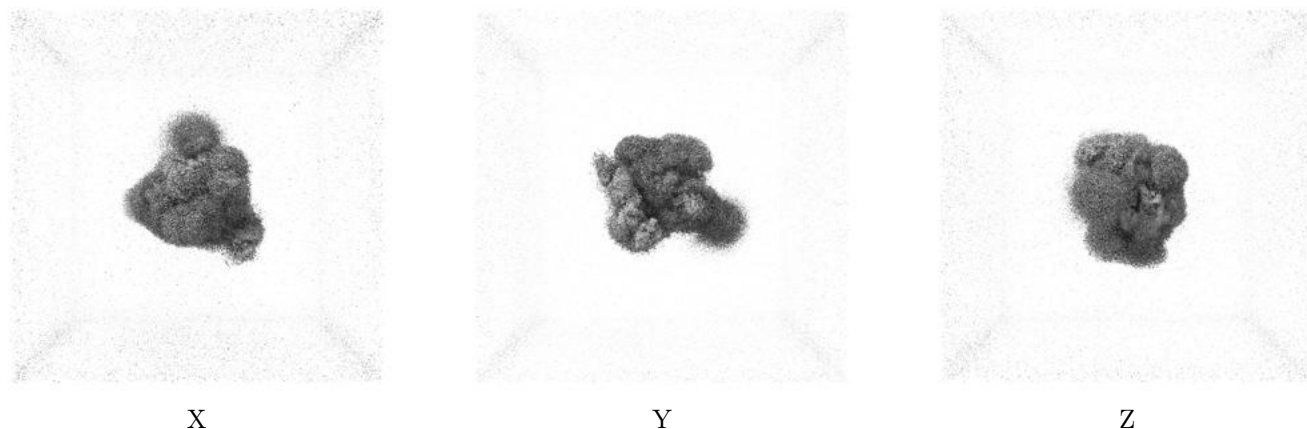


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

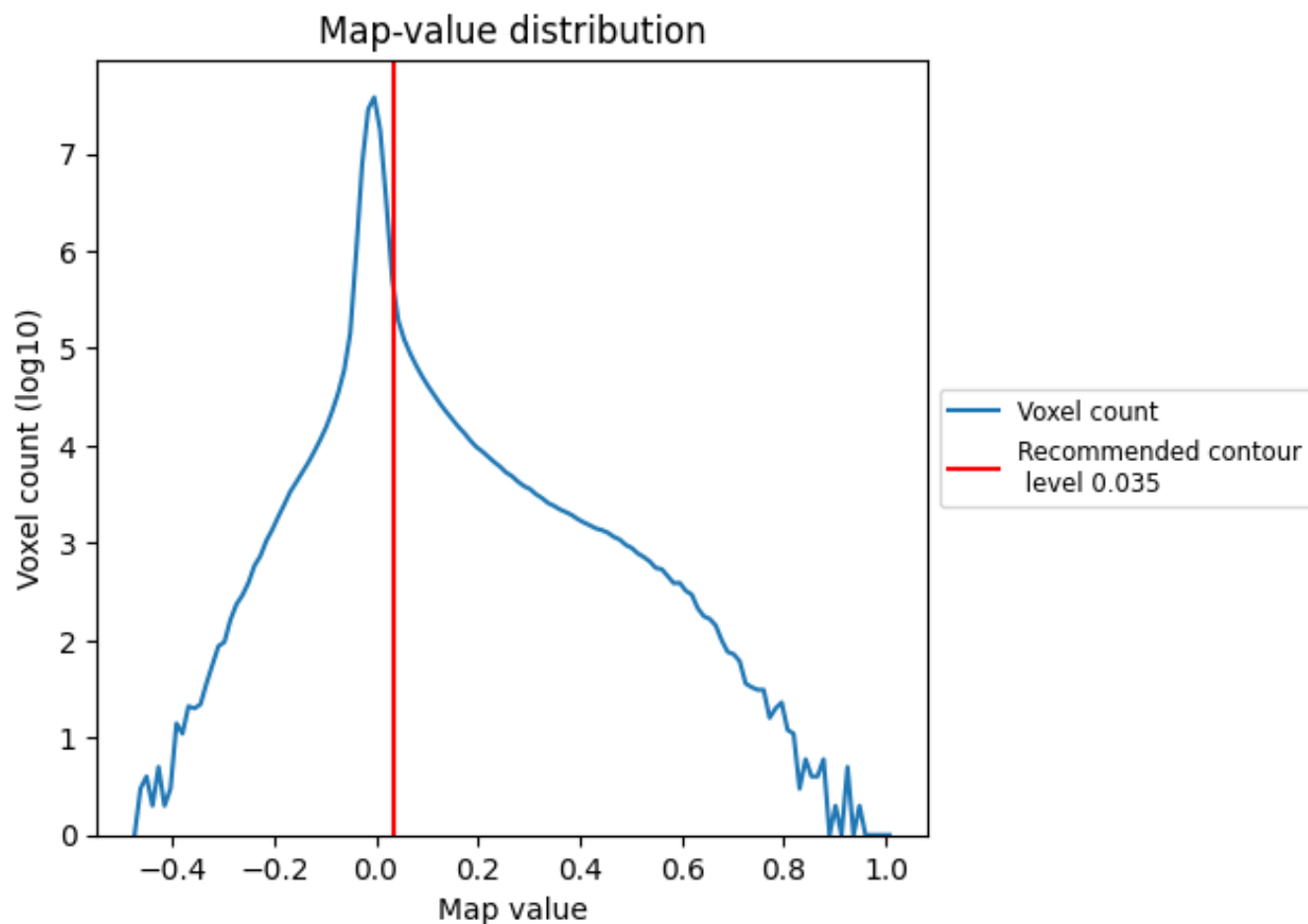
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

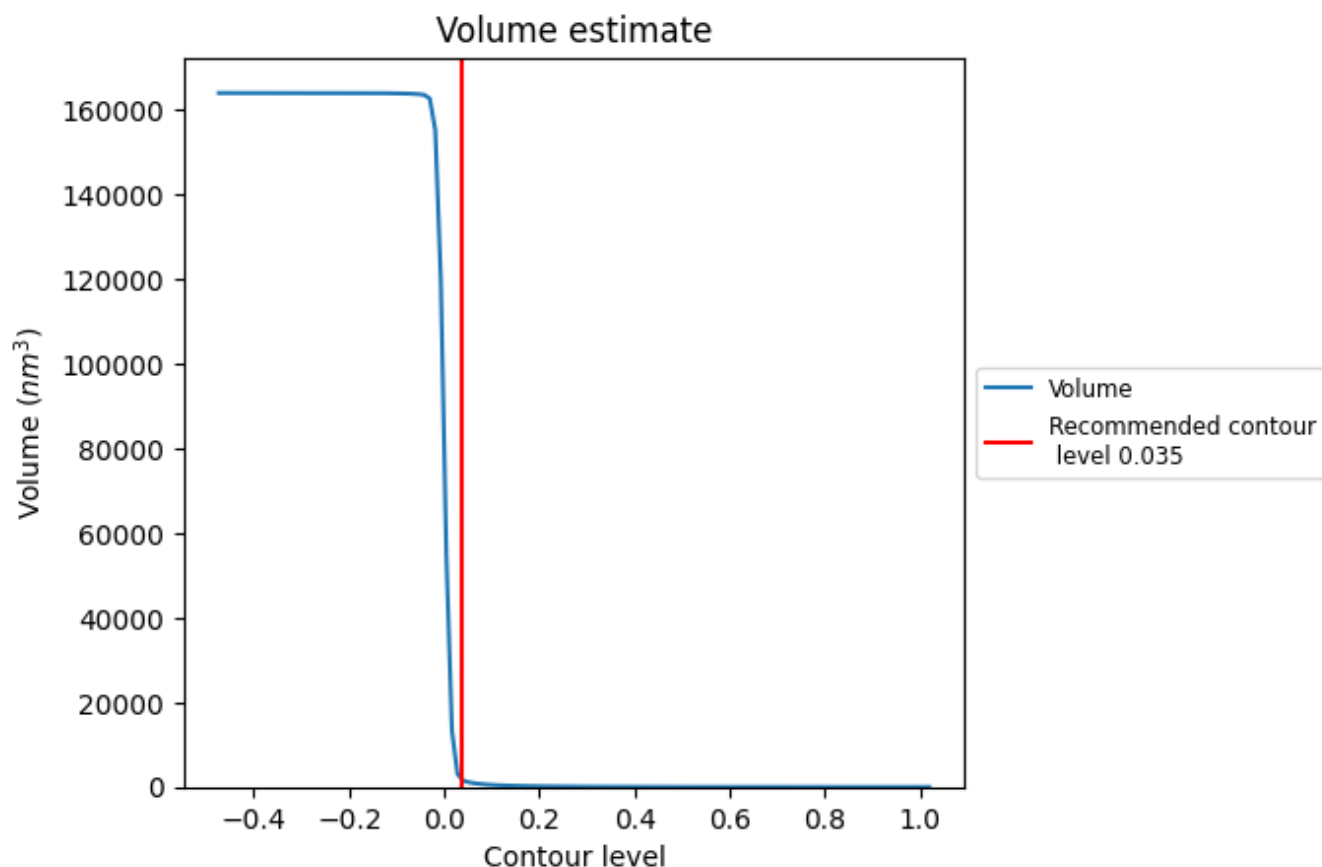
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

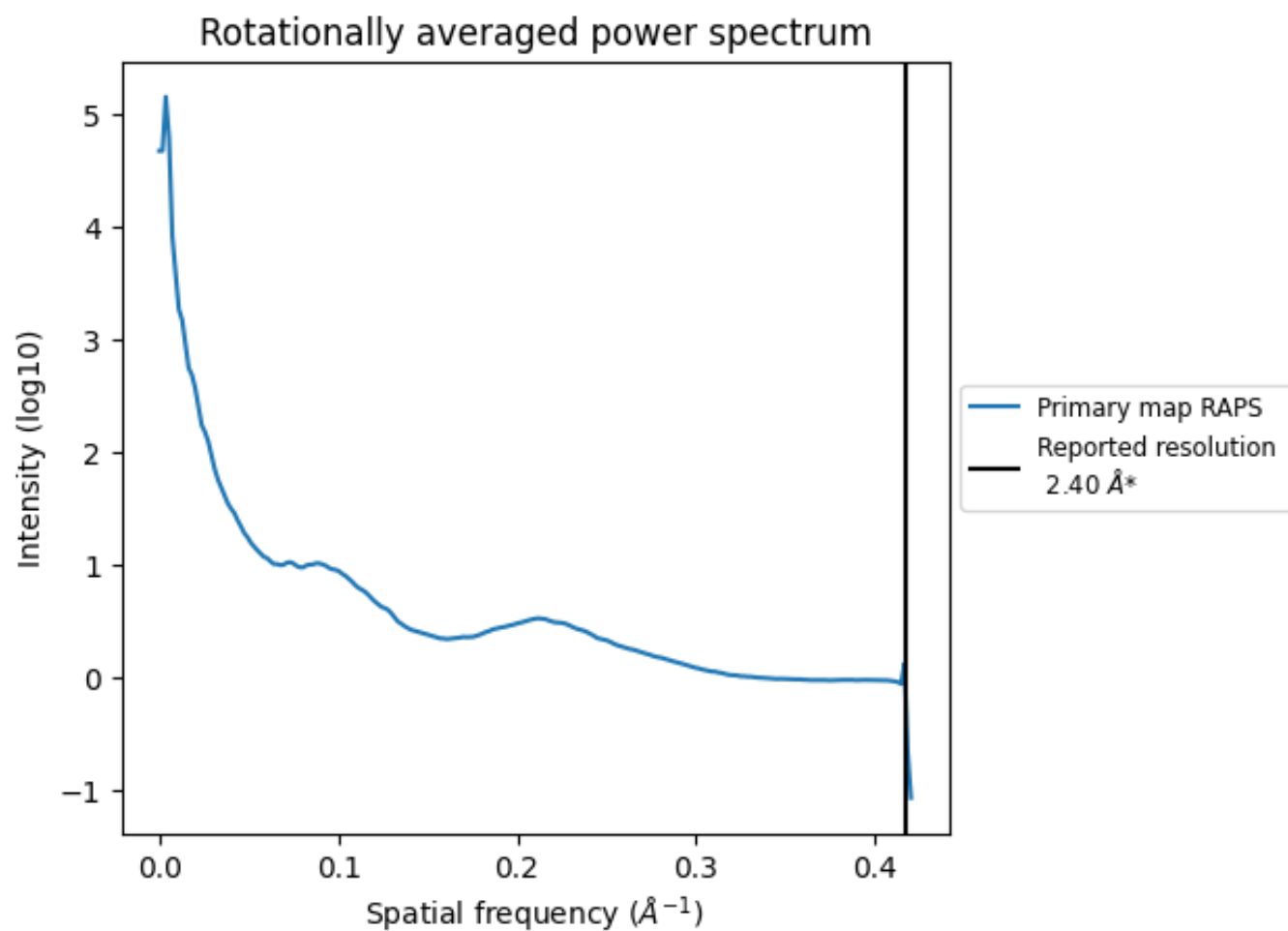
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2127 nm^3 ; this corresponds to an approximate mass of 1922 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

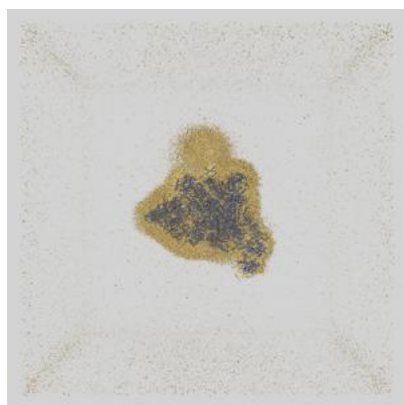
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

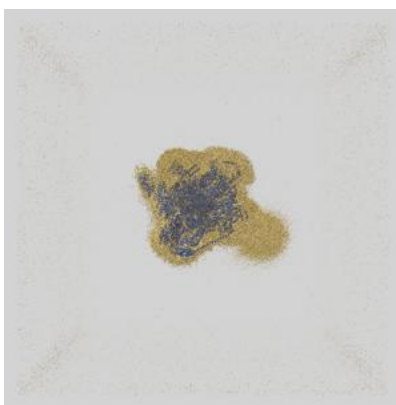
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48353 and PDB model 9MLC. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

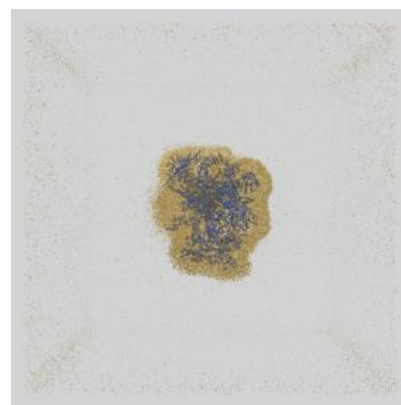
9.1 Map-model overlay [i](#)



X



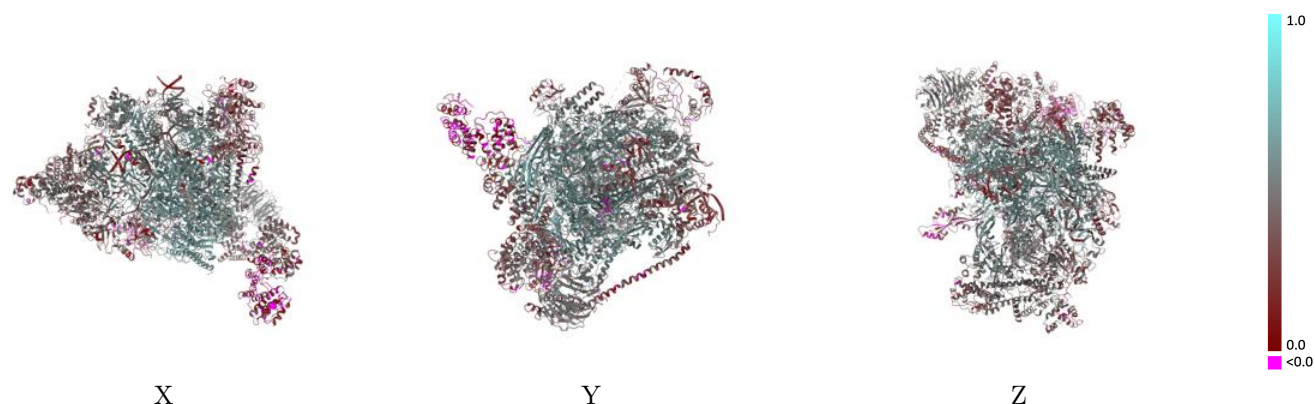
Y



Z

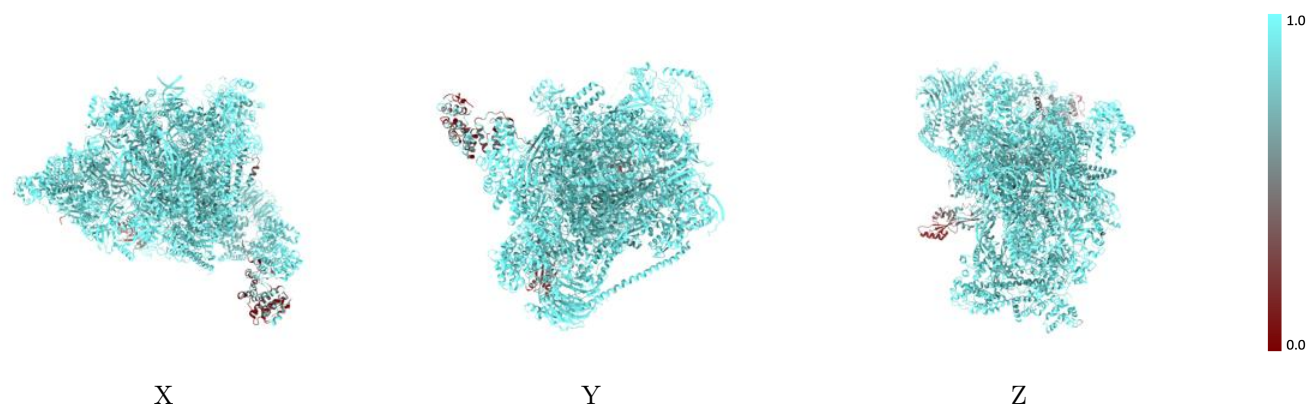
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



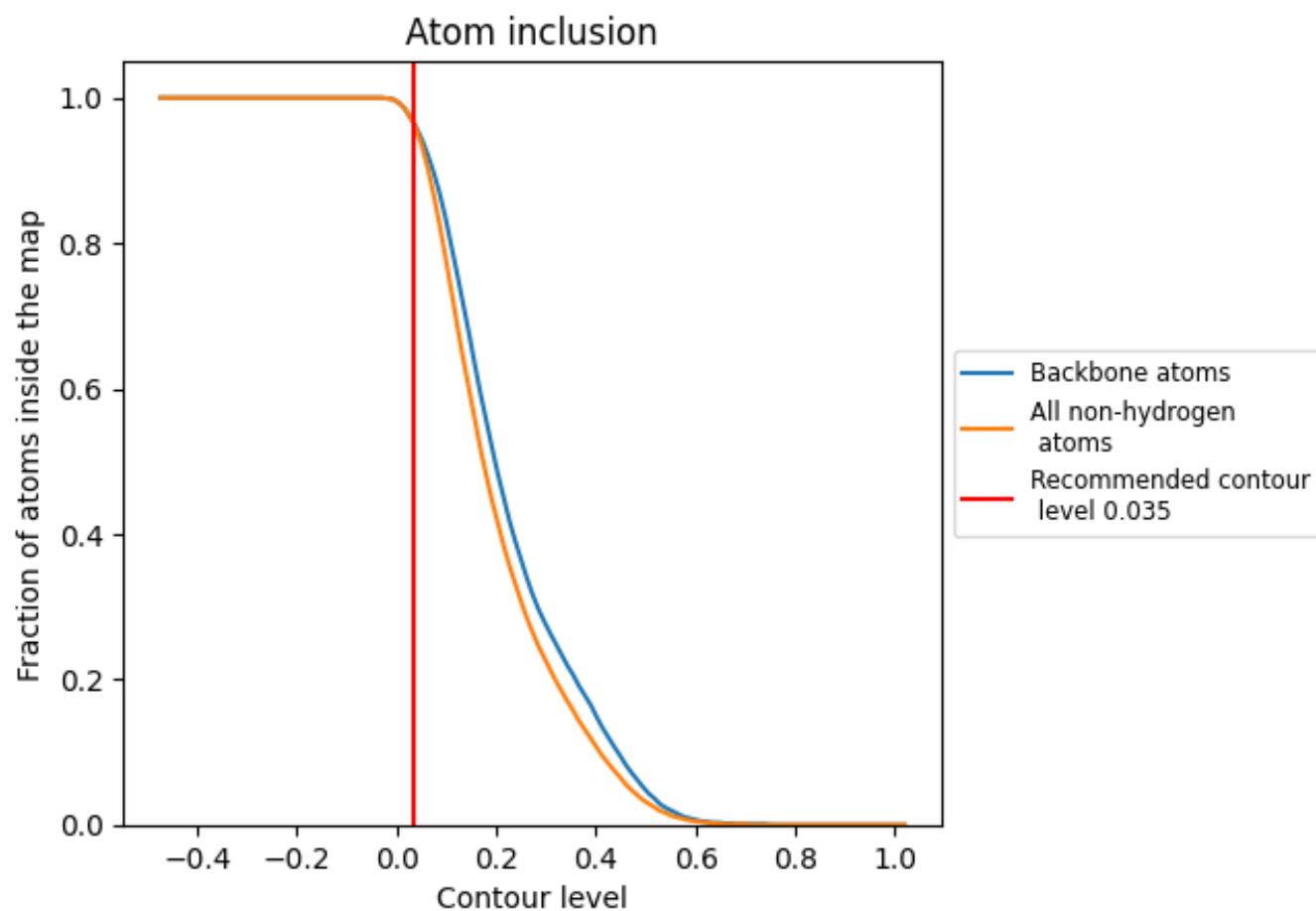
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4680
A	 0.9850	 0.5600
B	 0.9850	 0.5680
C	 0.9960	 0.6060
D	 0.9710	 0.4350
E	 0.9930	 0.5290
F	 0.9800	 0.5960
G	 0.9820	 0.5390
H	 0.9850	 0.5850
I	 0.9600	 0.2920
J	 0.9860	 0.5990
K	 0.9980	 0.6200
L	 0.9870	 0.5370
M	 0.9180	 0.3620
N	 0.9880	 0.3110
O	 0.9710	 0.4990
P	 0.9930	 0.4630
Q	 0.9020	 0.3050
R	 0.9530	 0.3900
S	 0.9580	 0.2660
T	 0.9830	 0.3950
U	 0.9890	 0.3370
V	 0.9380	 0.3270
W	 0.9810	 0.4490
X	 0.8790	 0.2850
Y	 0.9830	 0.4950
Z	 0.9800	 0.4810
i	 0.9480	 0.4280

